Spatial Inhomogeneity and Thermodynamic Chaos

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Abstract: We present a coherent approach to the competition between thermodynamic states in spatially inhomogeneous systems, such as the Edwards-Anderson spin glass with a fixed coupling realization. This approach explains and relates chaotic size dependence, "dispersal of the metastate", and for replicas: non-independence, symmetry breaking, and overlap (non-)self-averaging.

The connection between the existence of many thermodynamic states and the phenomena of non-self-averaging (NSA) and replica symmetry breaking (RSB) has long been a central topic of research in disordered systems. These phenomena play a key role in Parisi's solution [1, 2, 3] of the infinite-ranged Sherrington-Kirkpatrick (SK) Ising spin glass model [4], and have been discussed in many other contexts, e.g., short-ranged spin glasses [5, 6], random field XY models [7], random manifolds [8], heteropolymers [9], and impure superconductors in magnetic fields [10]. Another aspect of the competition between thermodynamic states, introduced by the authors in Ref. [11], is "chaotic size dependence" (CSD) which, unlike NSA, manifests itself for a fixed realization of the disorder.

An important issue is whether (and in what sense) the many novel features of Parisi's solution can apply to more realistic models, such as the Edwards-Anderson (EA) nearest-neighbor Ising spin glass [12]. In a previous paper [13], it was shown that this "SK picture", as conventionally understood, is not valid. In particular, the overlaps of the thermodynamic states for coupling realization $\mathcal{J}$ do *not* depend on $\mathcal{J}$. This leads us to approach all basic phenomena as accessible for a *fixed* realization. Although we focus here on disordered systems, this approach is applicable to the more general setting of inhomogeneous systems.

We shall see that CSD is one aspect of a phenomenon, "dispersal of the metastate", which is closely connected with both NSA and RSB. The metastate is a natural ensemble, i.e., a probability measure, on the (pure or mixed) thermodynamic states of the system [14]. At high temperature, it is a δ-function on a single state; we call this a non-dispersed

*Partially supported by the National Science Foundation under grant DMS-95-00868.
†Partially supported by the U.S. Department of Energy under grant DE-FG03-93ER25155.

metastate. CSD will occur if the metastate ceases to be a single δ-function; we call this a dispersed metastate. It will become apparent below, but we emphasize now, that *dispersal of the metastate is not the same as the mere existence of many states*. One unfamiliar but essential feature of our approach is a replacement for the usual notion of NSA; we shall see that (unlike the standard SK picture) *replica overlap fluctuations (if they occur) are due not to explicit $\mathcal{J}$-dependence but rather to state-dependence within the metastate for fixed $\mathcal{J}$.*

We also find further connections between the structure of the metastate and that of the replicas: dispersal of the metastate is equivalent to *replica non-independence* (RNI), to be explained below, while RSB is equivalent to the individual states in the metastate being mixtures (of pure states).

CSD and the metastate. — A thermodynamic state Γ of a system such as the EA model at temperature T with fixed $\mathcal{J}$ (we take zero magnetic field) is in general a mixture of pure (extremal) states. If there are many pure states, e.g., as predicted by the SK picture [15], CSD could occur [11]. This would mean that for finite volume Gibbs states with $\mathcal{J}$-independent boundary conditions, such as $\rho^{(L)}$ (with periodic b.c.'s on the L^d cube Λ_L centered at the origin), the correlations $\langle \sigma_{i_1} \ldots \sigma_{i_m} \rangle_L$ will have no single limit as $L \to \infty$ but rather many different limits along different subsequences of L's.

Such behavior in L is analogous to chaotic behavior in time t along the orbit of a dynamical system. In both cases, the dependence of the state (on L or t) is actually deterministic but appears to be a random sampling from some distribution κ on the space of states. For inhomogeneous or disordered systems, κ is a metastate, i.e., a probability measure on the space of all (fixed $\mathcal{J}$) thermodynamic states, and is the limit of κ_L, a "microcanonical" ensemble in which each of the finite volume states $\rho^{(1)}, \ldots, \rho^{(L)}$ has weight L^{-1}. The meaning of the limit is that for every (nice) function g on states (i.e., a function of finitely many correlations),

$$\lim_{L\to\infty} L^{-1} \sum_{\ell=1}^{L} g(\rho^{(\ell)}) = \{g(\Gamma)\}_\kappa \quad . \tag{1}$$

Here, the bracket $\{.\}_\kappa$ denotes the average over κ.

What are some possibilities for the metastate κ in the EA model? If there is a unique thermodynamic state there is no CSD and κ is not dispersed – it is a δ-function on that state. If (as in the Fisher-Huse (FH) droplet picture of the spin glass phase [16, 17]) there is only a pair of pure states, related by a global spin flip, then κ is a δ-function on the equal-weight mixture of these two states; there is still no CSD and no dispersal of κ, even though the pure states break spin flip symmetry. On the other hand, a *dispersed* metastate would result if the periodic b.c.'s in Eq. (1) were replaced by, say, plus b.c.'s – namely, the equal-weight sum of the two δ-functions on each of the two pure states. The CSD yielding this metastate simply corresponds to the strong preference, for most large L's, of plus b.c.'s for one or the other (chaotically depending on L) of the two pure states. The possibilities in the EA model if there are many pure states will be discussed later; these include both dispersed and non-dispersed metastates.

What is NSA? — For disordered systems, there is an alternate construction of metastates,

due to Aizenman and Wehr [14]. The microcanonical ensemble κ_L is replaced by the ensemble of states on Λ_L obtained by varying the couplings outside Λ_L. The limit here means that for every (nice) function F of finitely many couplings and finitely many correlations,

$$\lim_{L'\to\infty}[F(\mathcal{J},\rho^{(L')})]_{av} = \Big[\{F(\mathcal{J},\Gamma)\}_{\kappa(\mathcal{J})}\Big]_{av} \quad . \tag{2}$$

Here, $[.]_{av}$ denotes the average over the (quenched) disorder distribution ν. The limit exists, for subsequences of L''s, and the resulting $\kappa(\mathcal{J})$ is a fixed-$\mathcal{J}$ metastate [14]. It can be shown (we will present a proof elsewhere) that for subsequences of ℓ's and L's, the limit in Eq. (1) exists and yields the *same* $\kappa(\mathcal{J})$. In both limits, the subsequences are $\mathcal{J}$-independent. We conjecture that actually all subsequences yield the same limiting $\kappa(\mathcal{J})$, which would then be *the* periodic b.c. metastate. For a different b.c., such as plus, there could be a different metastate, as noted above.

When F is chosen so as to fix the value of all couplings inside Λ_L and then $L \to \infty$, the RHS of Eq. (2) reduces to that of Eq. (1). Averaging over κ for fixed $\mathcal{J}$ thus corresponds to averaging over the "couplings at infinity". In realistic systems, thermodynamic state observables can depend on the bulk couplings and/or on the couplings at infinity. Thus we suggest that *there are two distinct types of dependence: (i) on $\mathcal{J}$, and (ii) on the state Γ within the metastate κ for fixed $\mathcal{J}$*. We shall see that replica overlaps cannot have the first type of dependence, but can in principle have the second kind. If overlap fluctuations (over the couplings) don't vanish as $L \to \infty$ [18], this is a signal that the *second* kind of dependence holds for infinite volume.

Replica Non-Independence — Suppose the functions $F(\mathcal{J},\rho)$ in the LHS of Eq. (2) are restricted to be linear in ρ, i.e., of the form $\langle f(\mathcal{J},\sigma)\rangle_\rho$. These determine a limit for the finite volume pair $(\mathcal{J}^{(L)},\sigma^{(L)})$, where $\mathcal{J}^{(L)}$ is the restriction of $\mathcal{J}$ to Λ_L and $\sigma^{(L)}$ is distributed by $\rho^{(L)}$. The limiting joint distribution is of the form $\nu(\mathcal{J})\rho_{\mathcal{J}}(\sigma)$ with $\rho_{\mathcal{J}}$ a fixed-$\mathcal{J}$ thermodynamic state [13, 19], which is simply the mean state (or barycenter) of $\kappa(\mathcal{J})$ [14] – i.e.,

$$\langle\sigma_{i_1}\ldots\sigma_{i_m}\rangle_{\rho_{\mathcal{J}}} = \{\langle\sigma_{i_1}\ldots\sigma_{i_m}\rangle_\Gamma\}_{\kappa(\mathcal{J})} \quad . \tag{3}$$

Guerra has pointed out [20] an important extension of this construction of $\rho_{\mathcal{J}}$. Take uncoupled (but identical) Hamiltonians for infinitely many replicas in finite volume, $\sigma^{1(L)},\sigma^{2(L)},\ldots$. This replaces $\rho^{(L)}(\sigma^{(L)})$ by the product measure $\rho^{(L)}(\sigma^{1(L)})\rho^{(L)}(\sigma^{2(L)})\ldots$, and leads to a limiting joint distribution for $(\mathcal{J}^{(L)},\sigma^{1(L)},\sigma^{2(L)},\ldots)$ of the form $\nu(\mathcal{J})\rho^\infty_{\mathcal{J}}(\sigma^1,\sigma^2,\ldots)$. Guerra further noted that nonvanishing of overlap fluctuations (as $L \to \infty$) should imply the non-interchangeability of taking (a) replicas and (b) the thermodynamic limit: $\rho^\infty_{\mathcal{J}}$ would *not* equal the product $\rho_{\mathcal{J}}(\sigma^1)\rho_{\mathcal{J}}(\sigma^2)\ldots$, but rather some mixture of products. In this case, one would have a Gibbs state $\rho^\infty_{\mathcal{J}}$ for the uncoupled replica Hamiltonians which is not simply the product of Gibbs states for the individual ones. The σ^i's in such a $\rho^\infty_{\mathcal{J}}$ would not be independent, but would be coupled implicitly through "boundary conditions at infinity". We call this non-independence among replicas RNI.

We raise two additional points here. The first is that replicas and the "replica state" $\rho^\infty_{\mathcal{J}}$ naturally follow (like $\rho_{\mathcal{J}}$) from the construction of the metastate $\kappa(\mathcal{J})$. The second is that

RNI is equivalent to dispersal of the metastate κ since the product decomposition of $\rho_{\mathcal{J}}^{\infty}$ is as a mixture over κ:

$$\rho_{\mathcal{J}}^{\infty}(\sigma^1, \sigma^2, \ldots) = \{\Gamma(\sigma^1)\Gamma(\sigma^2)\ldots\}_{\kappa(\mathcal{J})} \quad . \tag{4}$$

Both points can be explained in terms of "metacorrelations". Like the usual correlations, $\langle\sigma_A\rangle_\Gamma$ (where σ_A denotes $\sigma_{i_1}\ldots\sigma_{i_m}$ for the set $A = \{i_1, \ldots, i_m\}$), these are generalized moments of arbitrary order m and they characterize κ:

$$\{g(\Gamma)\}_\kappa = \{\langle\sigma_{A_1}\rangle_\Gamma \ldots \langle\sigma_{A_m}\rangle_\Gamma\}_\kappa \quad . \tag{5}$$

Restricting to $m = 1$ such g's in Eq. (1) (or the corresponding F's in Eq. (2)) yields $\rho_{\mathcal{J}}$ as explained above. Restricting to $m \leq 2$ such g's or F's yields the two-replica measure $\rho_{\mathcal{J}}^2(\sigma^1, \sigma^2)$ (corresponding to "integrating out" all the other replicas in $\rho_{\mathcal{J}}^{\infty}$), etc. Thus for any m, the correlation $\langle\sigma_{A_1}^1 \ldots \sigma_{A_m}^m\rangle$ evaluated in $\rho_{\mathcal{J}}^{\infty}$ equals the LHS of Eq. (5) evaluated in $\kappa(\mathcal{J})$. This proves Eq. (4).

Eq. (4) shows that RNI and RSB are distinct phenomena and either one can occur without the other. The former corresponds to a dispersal of κ over multiple Γ's, the latter to an individual Γ being a mixture of multiple pure states.

Overlaps. — A basic construct in Parisi's solution [15] of the SK model is the overlap distribution. For configurations σ, σ' on all space, the overlap should be defined as

$$Q(\sigma, \sigma') = \lim_{L\to\infty} L^{-d} \sum_{x\in\Lambda_L} \sigma_x \sigma'_x \quad . \tag{6}$$

Its distribution depends of course on how σ and σ' are chosen. If they are independently chosen from *pure* states [15], labelled α and β, then $\sigma_x\sigma'_x$ in Eq. (6) may be replaced by $\langle\sigma_x\rangle_\alpha\langle\sigma'_x\rangle_\beta$, and $Q = q^{\alpha\beta}$ with distribution $\delta(q - q^{\alpha\beta})$. In the standard SK picture, σ and σ' are chosen from the product measure $\rho_{\mathcal{J}}(\sigma)\rho_{\mathcal{J}}(\sigma')$. Ref. [13] proved that this picture is not valid for realistic models because the resulting overlap distribution does not depend on $\mathcal{J}$.

However, Guerra's work [20] and that of the previous section indicate that the standard SK picture should be replaced by one where σ and σ' (and other replicas) are taken from $\rho_{\mathcal{J}}^{\infty}$. Before we discuss various features of this nonstandard SK picture, we will now see that *the overlap structure still does not depend on $\mathcal{J}$.*

The overall overlap structure, given here by the (joint) distribution $P_{\mathcal{J}}^{\infty}$ for overlaps, $Q^{ij} = Q(\sigma^i, \sigma^j)$, between *all* pairs of replicas, contains much information. The simplest piece of information is the (marginal) distribution of a single overlap, say q^{12}; by Eq. (4), this equals $\{P_\Gamma(q^{12})\}_{\kappa(\mathcal{J})}$, where $P_\Gamma(q)$ denotes the overlap distribution coming from $\Gamma(\sigma)\Gamma(\sigma')$. More generally, the distribution for $Q^{12}, Q^{34}, Q^{56}, \ldots$ is

$$P_{\mathcal{J}}^{*}(q^{12}, q^{34}, \ldots) = \{P_\Gamma(q^{12})P_\Gamma(q^{34})\ldots\}_{\kappa(\mathcal{J})} \quad . \tag{7}$$

This shows that $P_{\mathcal{J}}^{\infty}$ can encode considerable information about the $\mathcal{J}$-dependent metastate κ, at least if different Γ's from κ yield distinct P_Γ's. Nevertheless, $P_{\mathcal{J}}^{\infty}$ (and hence $P_{\mathcal{J}}^{*}$) does not depend on $\mathcal{J}$. The proof is essentially the same as that given in Ref. [13].

Scenarios for the EA metastate. — We previously discussed the two possibilities for the EA model that the (periodic b.c.) metastate κ is 1) a δ-function on a single pure state or 2) a δ-function on a mixture of two pure states. If there are many pure states, other scenarios are possible. In all of these it is convenient to imagine that for large L, $\rho^{(L)}$ is approximately a mixture, $\sum_\alpha W_L^\alpha \rho^\alpha$, of pure thermodynamic states labelled by α (we suppress the fixed-$\mathcal{J}$ subscript in this section); the scenarios differ in how the weights W_L^α depend on α and L. Note that (for periodic b.c.'s) the ordered (i.e., with broken spin flip symmetry) pure states always come in pairs with $W_L^{-\alpha} = W_L^\alpha$.

One scenario is that $W_L^* \equiv \max_\alpha (W_L^\alpha + W_L^{-\alpha}) \to 0$ as $L \to \infty$. Then each state Γ from κ should have an integral (rather than sum) decomposition, $\Gamma = \int W_\Gamma(\alpha) \rho^\alpha d\alpha$. There are then two possibilities, both of which exhibit RSB: either 3) there is no CSD (or RNI) and κ is a δ-function on a single such Γ or 4) there is CSD (and RNI) and κ is a dispersed measure over many such Γ's (and $W_\Gamma(\alpha)$'s). Both possibilities would be quite unlike either the SK or FH pictures; competition between pure states would be so well matched that for most large L's, no group of a few states dominates.

On the other extreme is the scenario where $W_L^* \to 1$ as $L \to \infty$ (we assume here that every ρ^α is ordered). This could occur without CSD (or RNI), which leads back to possibility 2, or else 5) there is CSD (and RNI) and κ is dispersed over many Γ's, each of the form $[\rho^\alpha + \rho^{-\alpha}]/2$. This latter possibility is an intriguing revision of the FH picture; the competition between pure states would be so mismatched that for most large L's, a single pair of states would dominate, but which pair would depend chaotically on L. Possibility 5 actually does occur in the ground state structure of a short-ranged, highly disordered spin glass model in high dimensions (while possibility 2 applies in low dimensions) [21]. Indeed, for the EA model itself at $T = 0$ (with a continuous distribution, such as Gaussian, for the individual couplings), only possibilities 2 or 5 can occur. We remark that in the plus b.c. version of possibility 5, there would be RNI but no RSB.

The nonstandard SK picture corresponds to an intermediate scenario where W_L^* tends neither to zero nor to one and most of the weight is concentrated on a few pure states, with the choice of states depending chaotically on L. In this possibility 6), there is CSD (and RNI) and κ is a dispersed measure over many Γ's, each with a sum decomposition, $\Gamma = \sum_\alpha W_\Gamma^\alpha \rho^\alpha$, so there is also (nontrivial) RSB. Such a Γ immediately yields the (fixed-Γ) overlap distribution

$$P_\Gamma(q) = \sum_{\alpha,\beta} W_\Gamma^\alpha W_\Gamma^\beta \delta(q - q^{\alpha\beta}) \quad . \tag{8}$$

The key objects of this picture are the P_Γ's and their average over κ, $P \equiv \{P_\Gamma\}_\kappa$. As noted, dependence on $\mathcal{J}$ and averaging over ν in the standard SK picture are replaced by dependence on Γ and averaging over κ. The basic requirements of this nonstandard SK picture are as follows: The fixed-Γ distribution $P_\Gamma(q)$ should be a countable sum of (many) δ-functions. This is a prerequisite for (nontrivial) ultrametricity within Γ, which is the second requirement. The third requirement is that the averaged distribution $P(q)$ be continuous between two δ-functions at $\pm q_{EA}$. We remark that the first and third requirements cannot both be valid unless P_Γ really does depend on Γ.

The nonstandard SK picture is the only way in which some familiar aspects of mean-field behavior can survive in the EA model, but it is not clear to us whether this picture is in fact valid in some dimensions at some temperatures. We do know that the overlap structure has no $\mathcal{J}$-dependence in both the standard and nonstandard SK pictures. This ruled out the standard picture [13]; we now pursue some implications for the nonstandard picture.

In addition to translation-covariance, the metastate $\kappa(\mathcal{J})$ is covariant with respect to changes ΔH of finitely many couplings (see Eq. (5.3) of Ref. [14]). Under such changes, pure states remain pure and the pure state overlaps $q^{\alpha\beta}$ do not change at all. However, the weights W_Γ^α, which appear in Eq. (8), will in general change. The overlap structure of Eq. (7) yields a measure on the set of weights appearing in the $P_\Gamma(q)$'s for each fixed set of possible $q^{\alpha\beta}$'s and by the lack of $\mathcal{J}$-dependence, each of these measures must be invariant under the change in weights created by every such ΔH. It is unclear whether the enormous number of constraints this imposes can be satisfied.

Discussion and conclusions. — For fixed $\mathcal{J}$, a metastate $\kappa = \kappa(\mathcal{J})$ is a probability measure on the fixed-T thermodynamic states Γ of the system. The Γ's can *a priori* be pure or mixed. For disordered systems, metastates were constructed by Aizenman and Wehr [14] by means of the ensemble of "couplings at infinity". The average $\{\Gamma\}_{\kappa(\mathcal{J})}$ over this metastate is the state $\rho_{\mathcal{J}}$ (independently constructed in [19]) used in [13] to rule out the standard SK picture for the EA model.

In this paper, we constructed the same metastate κ, but by means of the ensemble of finite volume states $\rho^{(L)}$ for a *fixed* $\mathcal{J}$, so that our approach can be applied to inhomogeneous systems in general. Dispersal of κ, if it occurs, implies chaotic size dependence of $\rho^{(L)}$. Furthermore, replica symmetry breaking is equivalent to the appearance of mixed states Γ in κ, while dispersal of κ is equivalent to replica non-independence (as introduced by Guerra [20]).

We then classified the principal behaviors which can occur, using the EA model as our prototype. Among the scenarios are possibilities 3 – 5, which are quite unlike any of the standard pictures.

Another new scenario (possibility 6), referred to as the "nonstandard SK picture", maximizes the features of mean field behavior that *might* survive in short-ranged models despite the elimination of the standard SK picture in Ref. [13]. In this picture, the thermodynamic state $\rho_{\mathcal{J}}^\infty$ on all replicas for *fixed* $\mathcal{J}$ can be written as an integral, over the Γ's of $\kappa(\mathcal{J})$, of independent Γ-distributed replicas (see Eq. (4)). Each Γ would be a weighted sum, $\sum_\alpha W_\Gamma^\alpha \rho_{\mathcal{J}}^\alpha$, from a *countably infinite* family of pure states, but the integral (given by κ) would be over a *continuum* of choices of these families (as well as over the weights for each family), all for a fixed $\mathcal{J}$. The measure κ prescribes the probability of obtaining both a particular family of pure states and their weights. This probability corresponds to selecting the family (and weights) according to $\rho^{(L)}$ with L large and chosen at random (but with $\mathcal{J}$ fixed); each different choice of L will in general select out a different family of pure states.

If such a picture holds, some familiar mean-field behavior would be exhibited in short-ranged models. In particular, one would find dominance of a few states in large finite volumes (but with the family from which they're chosen changing chaotically with volume).

A restricted (within Γ) ultrametricity of overlaps is not ruled out, but the countable nature of each Γ places strong constraints on the nature of the metastate.

We emphasize that the nonstandard SK picture differs from the usual one in important respects. In particular, there is no dependence of overlap distributions on $\mathcal{J}$, but only on the state Γ within κ. Also, ultrametricity would not hold in general among any three pure states [13], but would be valid only for states from the same Γ.

We have previously shown [13] that short-ranged models display non-mean-field behavior; i.e., the existence of a $\mathcal{J}$-dependent state $\rho_{\mathcal{J}}$ with $\mathcal{J}$-independent overlaps. If some of the more familiar mean-field properties are nevertheless to hold for the thermodynamic states, then something like our nonstandard SK picture must be present. But this picture is very heavily constrained. The probability distribution on weights of pure states and their overlaps *cannot change with* $\mathcal{J}$; in particular the distribution on weights must be invariant with respect to any changes of any finitely many couplings. Whether this is reasonable can be judged by the reader; whether it will survive must be determined by future work.

Acknowledgments. The authors thank M. Aizenman and A. van Enter for useful conversations; they also gratefully acknowledge an extremely stimulating correspondence with F. Guerra.

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